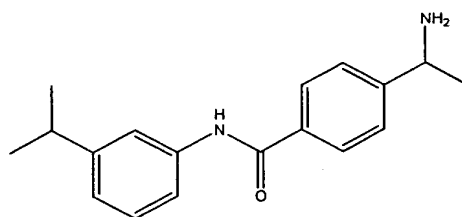


09085893-062001



A

6  
269.80 2 5 4 1 3 BTB\_03049  
229.80 6 5 1 2 4 SPB\_00387  
259.85 4 3 2 1 1 EN\_00236  
179.05 4 2 0 0 2 NRB\_00265

B

Fig. 1

```
graph TD; A["Molecule Data Base  
(40,000 molecules Mi)"] --> B["Calculating 6-dimensional descriptor Xi for  
each molecule Mi"]; B --> C["Selecting arbitrarily  
400 molecules Mi  
as initial population  
(subset Su)"]; C --> D["Genetic Algorithm  
(Fig. 2 B)"]; D --> E["Outputting the molecules Mi of Su  
ordered by their fitnesses f(Mi)"]; E --> F([End]);
```

The flowchart illustrates the process of selecting molecules for a genetic algorithm. It begins with a 'Molecule Data Base' containing 40,000 molecules  $M_i$ , represented by a parallelogram. Two chemical structures are shown: benzylbenzene (c1ccccc1Cc2ccccc2) and 1-phenylpropane (CC(c1ccccc1)C). The process then moves to a rectangular box for 'Calculating 6-dimensional descriptor  $X_i$  for each molecule  $M_i$ '. This is followed by another parallelogram for 'Selecting arbitrarily 400 molecules  $M_i$  as initial population (subset  $S_u$ )'. The next step is a rectangular box for the 'Genetic Algorithm (Fig. 2 B)'. This leads to a final rectangular box for 'Outputting the molecules  $M_i$  of  $S_u$  ordered by their fitnesses  $f(M_i)$ '. The process concludes with an oval labeled 'End'.

Fig. 2A

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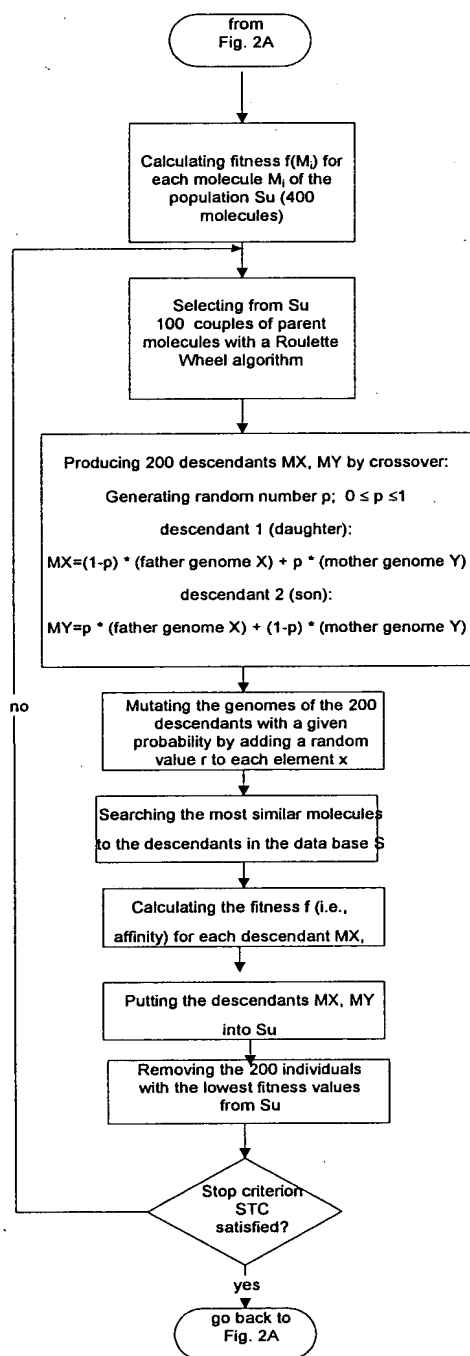


Fig. 2B

attribute	1	2	3	4	5	6	
father genome X	0,7	0,4	0,1	0,5	0,2	0,9	Sum = 5,8
mother genome Y	0,5	0,8	0,6	0,1	0,5	0,5	
descendant 1 (son)	0,54	0,72	0,5	0,18	0,44	0,58	Sum = 5,8
descendant 2 (daughter)	0,66	0,48	0,2	0,42	0,26	0,82	

$\text{son} = p \times (\text{father\_genom}) + (1-p) \times (\text{mother\_genom})$   
 $\text{daughter} = (1-p) \times (\text{father\_genom}) + p \times (\text{mother\_genom})$

$p=0.2$

Fig. 3

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T00290" C6858860

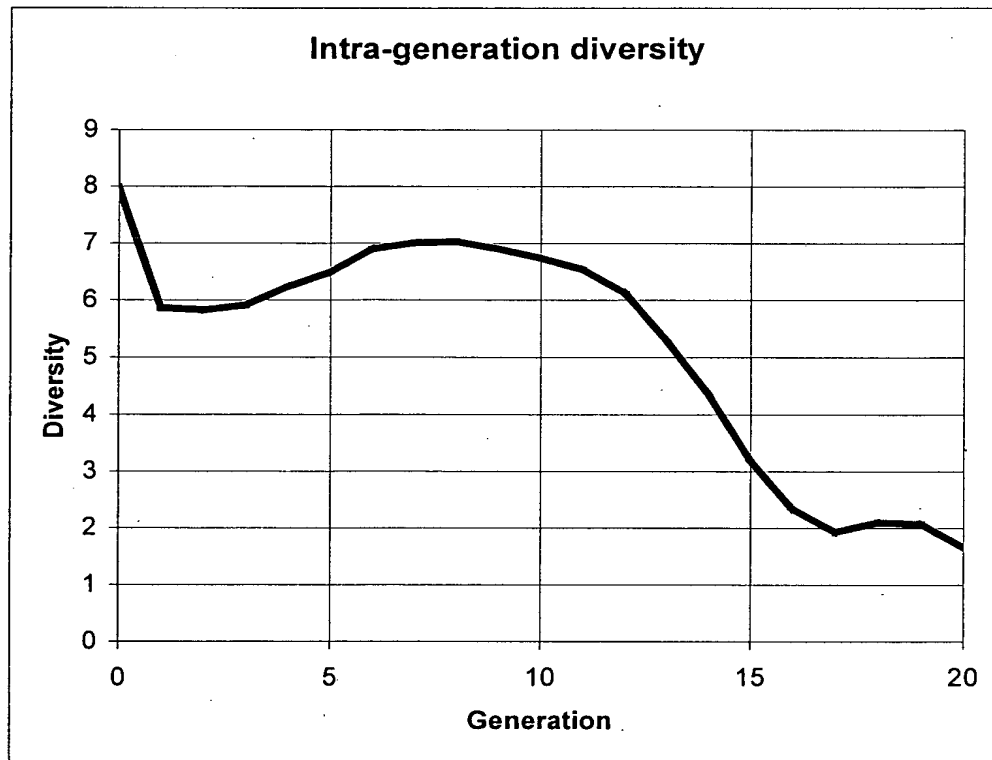


Fig. 4

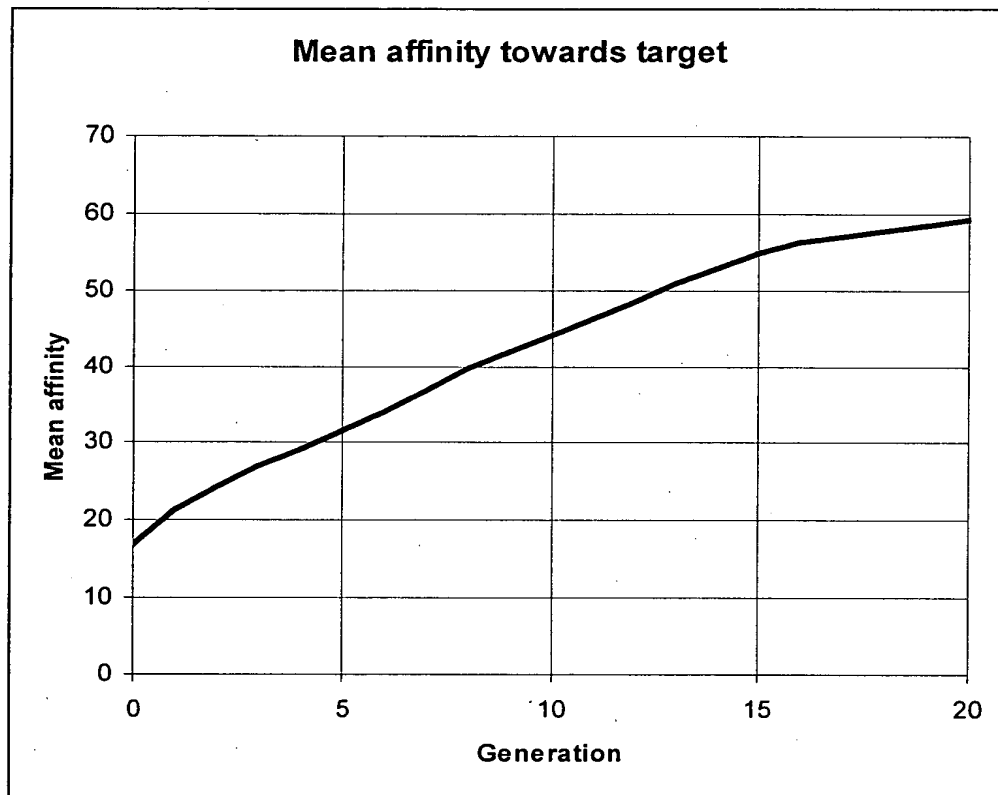
[illegible]

Fig.5

098583 02001  
F00290" E6858360

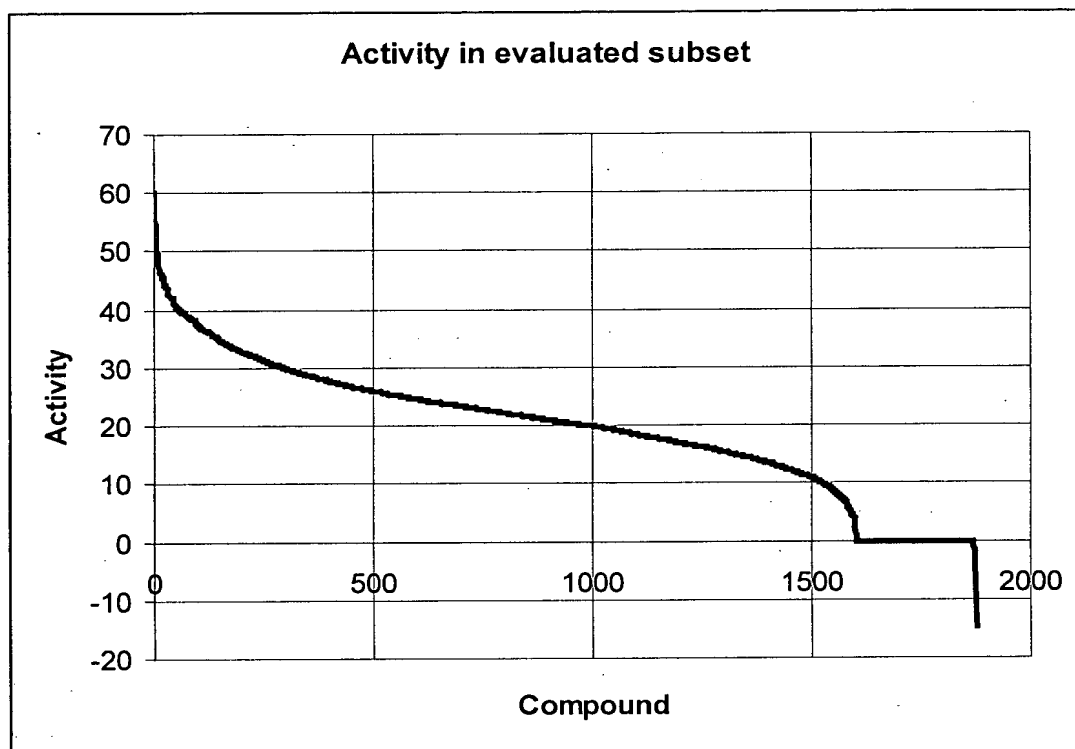


Fig. 6

FO0290" C6858860

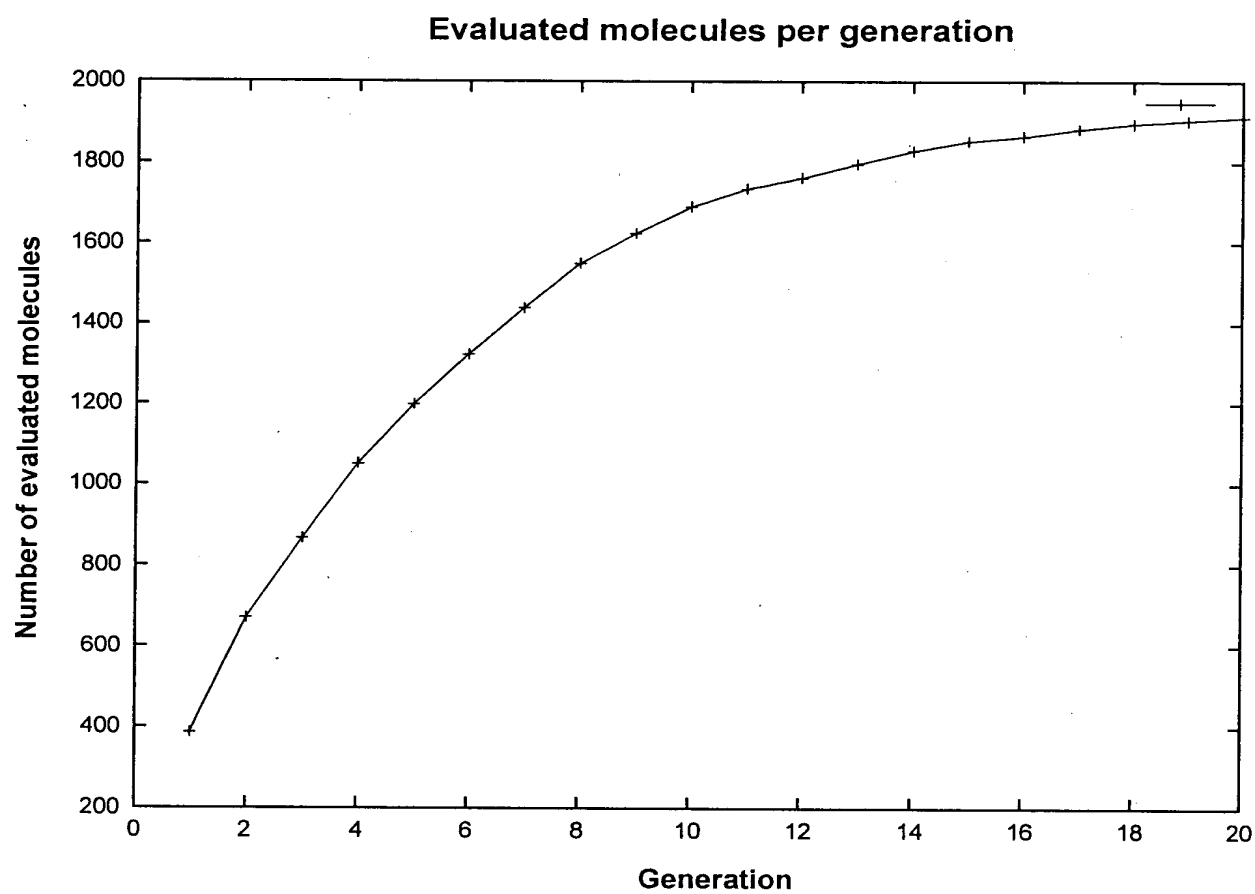


Fig. 7